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Tight-binding Calculation of Electronic Properties of Oligophenyl and Oligoacene Chains ADAM HINKLE, ANTONIO C. CANCIO, MAHFUZA KHATUN, Ball State University — Within recent years, allotrophic structures of carbon have been produced in the forms of tubes and ribbons which offer the promise of extraordinary electronic and thermal properties. Here we present analyses of oligophenyl and oligoacene systems– -infinite, one-dimensional chains of benzene rings linked along the armchair and zigzag directions. These one-dimensional structures, which are amenable to calculation by analytical means, exhibit features very similar to carbon nanotubes and nanoribbons. Using a tight-binding Hamiltonian we analytically determine the energy bands of these systems. From these results we calculate the density of states and wavefunction symmetries for each structure. We also discuss the effect doping has on the energy as well as examine the transport properties.

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